# NCNR

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## MACS List of Requirements

This document defines the top-level specification for **M**ulti **A**xis **C**rystal **S**pectrometer, MACS, at NG0 of the NIST reactor (NBSR). The document becomes effective only if all parties whose names appear below have signed it. Changes to the signed document can be initiated by each of those parties, or their replacements, at which time a new document including the proposed revision is prepared. Changes become effective only after all parties sign the new document. Newly modified sections shall be marked as such. The old document remains part of the record.

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# Requirements for MACS.(1)

## 1. Beam extraction system

### 1.1 Beam tube dimensions (modified)

The aperture at $L_a$=1654 mm from the source shall be left open. The beam tube opening following this aperture shall be minimized while ensuring that the $w_m$ x $h_m$ = 441 mm x 357 mm monochromator when in monochromatic focusing geometry is illuminated as much as possible throughout the range of incident energies considering the afore mentioned aperture. For this optimization, the active part of the source shall be taken to be the geometrical optical image on the source of a 20 mm wide by 40 mm tall sample located on the sample table.

### 1.2 Beam line shielding and atmosphere (New)

From source to sample the beam path shall be evacuated or filled with $^4$He wherever feasible to minimize air scattering losses. All space which is not part of the active beam tube as specified by 1.1, shall to the extent feasible, be filled with neutron shielding material. There are two exceptions to this: Shielding around the monochromator that can be viewed from the sample position shall be recessed so that it is not illuminated by the reactor beam. Furthermore, the location and characteristics of the reactor beam dump shall be chosen to minimize its contribution to the detector count rate.

### 1.2 Shutter (modified)

The beam shutter shall be outside the biological reactor shielding. It must reduce radiation incident on the monochromator sufficiently to allow extraction of a monochromator for repairs while the reactor is operating. It must also reduce radiation on the sample to less than 5 mR/hr when closed. The time to open or close shall be less than 15 sec. A clearly visible sign shall indicate the position of the shutter and this information shall be available to the instrument control computer. The shutter position shall be controlled from a single switch that is interlocked with a radiation exclusion zone, details of which are to be specified by NIST health physics.

### 1.3 Pre monochromator filters (modified)

There shall be a 3-position filter exchanger immediately following or part of the shutter mechanism. All filters shall be large enough in their transverse dimensions to accommodate the full beam as specified in 1.1. Shielding material shall surround each filter such that neutrons either pass through the filters or are absorbed in the surrounding shielding. All filters shall be cooled to 77 K or colder and remain at that temperature when fully illuminated by the reactor beam. Filter changes shall be effectuated from the instrument control computer. Filter options shall be:

**1.3.1 (modified)** Single crystalline sapphire grade B4 or better from Crystal Systems Inc. with a beam path length of 80 mm. The orientation of the single crystalline material shall be uniform throughout the filter to within 10 degrees. However, the average crystal orientation with respect to the beam direction is unimportant and shall be chosen to minimize cost.

**1.3.2 (modified)** Beryllium grade I-220-H from Brush Wellman with a beam path length of 100 mm.

**1.3.3 (modified)** Pyrolytic Graphite grade ZYH from Advanced Ceramics with a total beam path length of 80 mm. The c-axis shall be oriented to within 2 degrees of the local beam direction back to the center of the source.

## 2. Monochromating system

### 2.1 General Principle (modified)

The monochromator design is based on a system in which the crystal slides along the white beam, while it rotates simultaneously. At the same time, a shielding drum holding a converging super-mirror guide rotates around an axis that is located on the line connecting the sample rotation axis and the current monochromator rotation axis. The sample position axis is permanently attached to this drum. The drum shall be tightly sandwiched between two saddle shields, yet be free to rotate. We denote the location of the monochromator at $2q_M = 90^0$ as the reference position. The distance from the reference position to the source, to the center of the drum, and to the sample shall be minimized while maintaining all other specifications.

### 2.2 Pre-monochromator collimators

**2.2.1 (modified)** Immediately following the filter exchanger shall be a 4-position collimator exchanger. Collimator changes shall be effectuated from the control computer. It shall take less than 30 sec. to exchange collimators. All collimators shall be embedded in neutron shielding material so that neutrons either pass through the window of the collimator or are absorbed. This shielding shall have high Boron content.

**2.2.2 (modified)** There shall be four different collimators. All shall be radial collimators with the source as their focal point. The window of the collimator shall match the size of the beam as specified in 1.1. The spacing between blades shall be given by

$$d = a\ell \frac{L_{0r}}{L_{0r} - L_{cr}},$$

where $L_{cr}$ is the distance from the center of the monochromator at its reference position to the down stream and broadest side of the collimator, $L_{0r}$ is the distance from monochromator reference position to source, and $\ell = 400$ mm is the length of the collimator blades. The thickness of the blades shall be 0.2 mm or less. The effective beam divergence, *a*, shall be 20', 40', 60', and 120' for the 4 collimators respectively.

**2.2.3** **(modified)** The focal point of the collimators shall coincide with the brightest part of the source to within 10 mm in the transverse directions and 100 mm in the longitudinal direction. The collimators shall be parallel to each other to within 0.03 degree. A line parallel to the central blade of any collimator shall pass through the monochromator rotation axis to within 5 mm.

**2.3 Variable Reactor Beam aperture (modified)**

As close as possible and no more than 1100 mm from the center of rotation of the active monochromator shall be a slit capable of closing the reactor beam from the dimensions specified in 1.1 to $w_{min}$=30 mm and $h_{min}$=50 mm. The aperture shall not be within line of sight of the sample in normal operation. The aperture shall be 100 mm thick, made from $B_4C$, and covered with LiF towards the reactor. The slit shall be centered with respect to the line connecting the monochromator rotation axis to the center of the source to within 2 mm.

**2.4 Monochromator exchanger (modified)**

This device shall enable computer-controlled selection between two different single crystal monochromator assemblies. Exchange shall take less than 1 minute. During typical operation, exchange will occur approximately once a week. The filling of this requirement may be combined with a translation stage specified in 2.1. It shall be possible to remove either one of the monochromators from the incident beam line for service during reactor operation.

**2.5 Monochromating assemblies (modified)**

There will be two doubly focusing monochromators. One based on pyrolytic graphite the other based on MICA, Heussler, Silicon, or Germanium to be specified at a later stage. The mechanical assemblies for each monochromator are specified separately. It shall be possible to extract both monochromating assemblies from the instrument for service while the reactor is operating. A web camera with appropriate lighting shall enable remote viewing of the monochromators for diagnostic purposed when they are driven to a specific position along the translation stage.

**2.6 Monochromator shield**

**2.6.1** Range of take-off-angles shall be 35° to 140°. It shall take less than 1 min. to change the take-off-angle from one extreme to the other. The monochromator translation stage and the drum rotation shall provide a setting accuracy of $0.03^o$ for the monochromator take off angle.

**2.6.2** **(modified)** Allowable radiation dose rate, and background, outside of monochromatic beam: ALARA. In addition, the instrument shall lie within an interlocked radiation exclusion zone that shall be separately specified in collaboration with NIST health physicists.

**2.7 Monochromator to sample super-mirror guide. (modified)**
From monochromator to sample shall be a converging super-mirror guide with the largest practical critical angle of order $3\theta^{Ni}_c$ . The guide shall extend from as close to the monochromator as possible until 250 mm before the sample. The inside height of the guide as a function of the distance, *x*, from the sample shall be given by

$$h(x) = h_S + \left(h_m - h_S\right)\left(1 - \frac{x}{L_{1r}}\right)$$

where $h_s$=40 mm is the sample height, $h_m$=357 mm is the monochromator height, and $L_{1r}$ is the monochromator to sample distance at the $2q_M$ =90$^o$ reference position. The sample end of the guide shall have an inside width of 18 mm and be centered with respect to the reference line that connects the sample rotation axis to the monochromator rotation axis to within 0.5 mm. The angle between the guide sides and the reference line shall be independently variable under computer control from 0 to 2.5$^o$ with an accuracy of 0.03$^o$. On either side of the guide where it protrudes from the monochromator drum shall be shielding that moves with the sides of the guide to function as beam defining apertures. On the sample end of the guide this shielding shall extend until the end of the guide and on the monochromator side it shall be as long as possible. The incoherent scattering cross section of materials that are illuminated by the monochromator and visible from the sample shall be minimized.

**2.8 Beam optics between super mirror guide and sample**
The following items shall be permanently mounted just after the super mirror guide. Their total thickness shall be less than 50 mm.

**2.8.1 (modified)** A monitor with a sensitivity no greater than $10^{-5}$ at 5 meV. The sensitivity shall be proportional to wave length.

**2.8.2 (modified)** An attenuation exchanger with four positions and capable of introducing three different planar objects into the beam under computer control. Two of the positions shall provide 10 times and 100 times attenuation respectively at 3.7 meV. These attenuators shall be permanently installed in the exchanger. The third position shall be an auxillary slot that can hold a plate with a thickness between 1 mm and 10 mm, width 40 mm and height 50 mm. When selected by the attenuation exchanger the plate shall be held in the center of the beam to within 1 mm. The attenuation exchanger shall be controlled from the main instrument control computer.

**2.8.3** A computer controlled thermal neutron aperture with variable opening from closed to the full width and height of the beam. The aperture shall be centered in the beam to within 0.5 mm and its degrees of freedom shall only be the width and height of the opening. The positioning accuracy shall be better than 0.5 mm.

## 3. Sample table

### 3.1 Location

The distance from the sample rotation axis to the monochromator rotation axis shall be minimized. When the spectrometer is in its $2q_M=90^o$ reference position this distance shall not be greater than 2500 mm.

### 3.2 Degrees of freedom provided. (modified)

**3.1.1** Rotation of sample 0-360$^o$ with accuracy of 0.005 degrees.

**3.1.2** Tilt of sample table +/- 12$^o$ about two mutually perpendicular horizontal axis. Accuracy better than 0.1$^o$ for loads in the range specified in 3.3. The effective rotation axes shall lie within 20 mm of beam height.

**3.1.3** Elevator +/- 20 mm about beam center. Accuracy better than 1 mm.

**3.1.4** Horizontal translation +/- 15 mm along two mutually perpendicular horizontal directions. Accuracy better than 0.5 mm. Translation shall occur along the sample tilt axes.

### 3.3 Dimensions and load capacity. (modified)

The mounting surface shall lie at least 152 mm below the beam center. Load capacity shall be 400 kg on axis. Max horizontal torque shall be 4 $10^2$ Nm and shall result in less than a 0.1$^o$ tilt of the sample rotation axis from the vertical.

## 4. Detection system

### 4.1 Specification for detector bank as a whole:

The detection system shall consist of at least 20 identical and equidistant detection "channels" which view the sample with a relative offset in scattering angle that shall be minimized and shall not exceed 8$^o$. The detection system shall cover 160$^o$ in the horizontal plane.

**4.1.1** The bank of detectors must be able to rotate as a whole around the sample such that the central detector covers the range of scattering angles from -45$^o$ to 45$^o$. The detector bank rotation shall be concentric with the sample rotation to within 0.5 mm. The setting accuracy shall be better than 0.01$^o$

**4.1.2** The effective scattering angle detected by each channel shall be within 0.03$^o$ of the nominal value

**4.1.3** It shall take less than 1 minute to rotate the detector bank between its extreme positions.

**4.1.4** The direct beam will always be incident on a part of the detector bank. Therefore, there must be a primary beam stop between the sample and the detector bank. The beam stop shall be as close to the detector bank as possible so it cannot scatter neutrons into active detection channels. The illuminated beam stop shall produce as little neutron and hard gamma radiation as possible. The width of the beam stop shall be minimized.

**4.1.5** **(modified)** A video camera with scintillating plate and image intensifier shall be available to position in front of any of the detection channels for radiography of the sample region or viewing Bragg reflected beams from the sample. The sensitivity shall allow real time imaging of 10,000-500,000 neutrons per second or integrated imaging of 1000 counts per second. The width of the camera at beam height shall be minimized. The images shall be available to the main computer for analysis and printing.

**4.2 Specification of individual detection channel:**

Each detection channel shall view a 20 mm wide by 40 mm tall sample with a horizontal divergence of at least 2 degrees and a vertical divergence of $8^o$. While the filters and collimator need not be independently selectable, the final energy setting of each channel must be. Each channel shall consist of the following items:

**4.2.1** **(modified)** Computer controlled selection of one of three different filters. All filters shall be cooled to a temperature of 77 K or less. Absorbing spacers shall prevent horizontal thermal neutron propagation by more than a channel width perpendicular to the beam. Filter options shall be 150 mm Thermalox 995 BeO machining stock from Brush Wellman. 100 mm Be with BW specification I220H Rev A type I from Brush Wellman. 50 mm Pyrolytic Graphite grade ZYH from Advanced Ceramics (PG). When in position each filter shall completely block the beam paths for all detection channels. Positioning of the filters with respect to each of the channels shall be reproducible to within 1 mm in all directions. PG filters must be oriented so that their crystallographic c-direction is within 1 degree of the average beam direction for the corresponding channel. The orientation of the PG filters shall be reproducible to within 0.1 degrees.

**4.2.2** **(modified)** computer controlled selection of three different collimators with divergence angles to be specified. The collimators shall be after the filters. The transmission of the collimators shall be greater than 90%.

**4.2.3** **(modified)** Double crystal PG(002) analyzer system covering the energy range from 2.5 meV to 15 meV. The width of the blades shall be 60 mm. The mosaic of each of the crystals remains to be specified. Starting from the sample, the first analyzer shall have a thickness of 4 mm and the second analyzer shall have a thickness of 2 mm. Both analyzers shall have fixed vertical focusing with a radius of curvature of 500 mm and their height shall be 180 mm.

**4.2.4** **(modified)** The angular accuracy for rotation shall be better than $0.03^o$ , which shall also be the reproducibility after 5000 motor movements. Translation of the analyzers shall be parallel to within $0.15^o$. The direction of translation for the first analyzer crystal shall coincide with the nominal centerline for the corresponding detection channel to within $0.03^o$ and 0.5 mm. The direction of translation for the second crystal shall be parallel to this direction to within $0.03^o$. The axis of rotation for each analyzer shall pass through the center of mass of the crystals to within 1 mm. The accuracy in placement of crystals on the cylindrically focusing surface shall be better than $0.3^o$ for analyzer number 1 and better than $0.15^o$ for analyzer number 2.

**4.2.5** **(modified)** It shall take less than 10 sec to change the final energy of all channels between their extreme limits and less than 2 sec to change the final energy of all analyzers by a FWHM of their energy resolution.

**4.2.6** There shall be two cylindrical $^3$He detectors associated with each channel. One immediately following the first crystal and viewing the sample through the collimator. One following the second crystal. Both detectors shall have a partial $^3$He pressure and thickness to achieve 90% detection efficiency for 15 meV neutrons over the full width of the detection channel. The height of the detectors shall be minimized under the constraint that they shall be tall enough to yield $8^o$ vertical acceptance taking into account the fixed vertical focusing of the crystals.

**4.2.7** **(modified)** Shielding shall be sufficient to yield a fast neutron background (measured by blocking the entrance to the channel with a cadmium sheet) of no more than 30 counts per hour per channel in the second detector over the full range of incident energies and configurations of the monochromating and analyzing system. The background in the first detector shall be less than 240 counts per hour under similar conditions.

**4.2.8** The energy resolution, integrated intensity, and fast neutron background shall vary by less than 10% from channel to channel. Background and integrated intensity shall vary less than 5% and mean energy less than 5 % of FWHM resolution following continuous use of the instrument for one month.

## 5 System Wide Requirements.

**5.1** **Hard and soft limits.** All degrees of freedom shall be equipped with soft and/or hardware limits that prevent any collisions but allow the full range of angles physically achievable. Sample rotation is a special case where hardware limits must be variable because of the different constraints associated with different sample environments.

**5.2** **Automated alignment.** There shall be an automated alignment protocol for all degrees of freedom of the instrument.

**5.3** **Permanent electrical wiring.** All wiring shall be permanently installed and comply with applicable industry standards.

**5.4** The instrument will require a dedicated and integrated **software package** to plan, execute, and analyze data to take optimal advantage of the doubly focusing monochromator and the multi-channel analyzing system. Details are to be specified separately.

**5.5** **Radiation Safety Exclusion zone.** In accordance with ALARA, the instrument shall be within an interlocked exclusion zone. No personnel can be in this zone when the beam is on. Details are to be specified by Health Physics.

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(1) Through the entire document metric units were used. Where standard stock sizes of materials will differ from the metric unit system, the closest four-digit decimal inch value will apply.